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An inversion algorithm for a banded matrix[☆]

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ABSTRACT

In this paper, an inversion algorithm for a banded matrix is presented. The n twisted decompositions of a banded matrix are given first; then the inverse of the matrix is obtained, one column at time. The method is about two times faster than the standard method based on the LU decomposition, as is shown with the analysis of computing complexity and the numerical experiments.

1. Introduction

The inverses of tridiagonal and banded matrices are necessary in solving many problems, such as computing the condition number, investigating the decay rate of the inverse and solving a linear system whose coefficient matrix is banded or tridiagonal. For banded matrices, there exist some investigations on the inverses of the matrices and the solution of the banded linear system, see [1–4]. For tridiagonal matrices, many efficient algorithms and explicit expressions of the elements of the inverse in some special cases for such inverse are presented, see [5–10].

In Meurant [6], the twisted decompositions of symmetric tridiagonal or block tridiagonal matrices are proposed to give the inverses of the matrices. In this paper, for a banded matrix subject to some conditions, a method for obtaining the inverse is presented. The results are related with n twisted decompositions of the banded matrix, which are first given in this paper. According to the jth twisted decomposition, the formulae for computing the jth column elements of the inverse are obtained. When we let $j = 1, 2, \dots, n$, a method is presented which inverts the banded matrix in order starting with the first column.

The standard method solves n linear systems for all the columns of the inverse, by using the LU decomposition. For convenience, it is denoted with LU method. From the analysis of the computing complexity, the method proposed is about two times faster than the LU method. Let p denote the bandwidth. Numerical experiments show that for $p \ll n$, the error of the proposed method is considerable smaller and the time complexity is likewise smaller than that for the LU method.

2. The inverse of banded matrices

Let $A = (a_{ij})$ be a nonsingular equal bandwidth matrix of order n such that $a_{ij} = 0$ if $|i - j| > p$, and $a_{ij} \neq 0$ if $|i - j| \leq p$, where p is a fixed positive integer such that $2p < n$. Obviously, the bandwidth of A is p. In general, many technical problems have a coefficient matrix with bandwidth p which is much less than n.

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Throughout the paper, it is assumed that all principal minors of A are nonzero.

In [11, p. 96], the LU decomposition of A is given, where the matrix L is a lower triangular matrix whose lower semi bandwidth is p and the matrix U is a upper triangular matrix whose upper semi bandwidth is p. Similarly, the UL decomposition can be given. Based on the two decompositions, we first give n twisted decompositions of the equal bandwidth matrix A. With the results in hand, we obtain simple and direct formulae for finding the inverse of A in order by column, starting with the first.

Theorem 2.1. *Let $A = (a_{ij})$ be a nonsingular equal bandwidth matrix of order n. For $j = 1, 2, \dots, n$,*
(i) *when $j = 1$, $A = UL$; when $j = n$, $A = LU$;*
(ii) *when $j = 2, \dots, n-1$, there exists a twisted decomposition such that $A = L_jU_j$, where*

$$L_j = \begin{pmatrix}
1 & & & & & & & & & \\
l_{21} & 1 & & & & & & & & \\
\vdots & \ddots & \ddots & & & & & & & \\
l_{p+1,1} & & \ddots & 1 & & & & & & \\
& \ddots & & l_{j,j-1} & 1 & l_{j+1,j} & \cdots & l_{j+p,j} & & \\
& & \ddots & \vdots & & \ddots & \ddots & & \ddots & \\
& & & l_{j+p-1,j-1} & & & \ddots & \ddots & & l_{n,n-p} \\
& & & & & & & \ddots & \ddots & \vdots \\
& & & & & & & & 1 & l_{n,n-1} \\
& & & & & & & & & 1
\end{pmatrix},$$

$$U_j = \begin{pmatrix}
u_{11} & \cdots\cdots & \cdots\cdots & u_{1,p+1} & & & & & \\
& \ddots & & & \ddots & & & & \\
& & \ddots & & & \ddots & & & \\
& & & u_{j-1,j-1} & \cdots & \cdots & u_{j-1,j+p-1} & & \\
& & & & u_{j,j} & & & & \\
& & & & u_{j,j+1} & u_{j+1,j+1} & & & \\
& & & & \vdots & \ddots & \ddots & & \\
& & & & u_{j,j+p} & & \ddots & \ddots & \\
& & & & & \ddots & & \ddots & \ddots \\
& & & & & & u_{n-p,n} & \cdots & u_{n-1,n} & u_{n,n}
\end{pmatrix},$$

and the sequences $\{l_{ij}\}$ and $\{u_{ij}\}$ may be obtained with the formulae:
1. *when $r = 1, 2, \dots, j-1$*
(1) $r = 1$

$$u_{ri} = a_{ri} \quad (i = 1, \dots, p+1), \qquad l_{ir} = \frac{a_{ir}}{u_{rr}} \quad (i = 2, \dots, p+1);$$

(2) $r = 2, \dots, j-1$
(a) *computing the rth row of U*

$$u_{ri} = a_{ri} - \sum_{k=\max(1,i-p,r-p)}^{r-1} l_{rk}u_{ki} \quad (i = r, \dots, r+p); \tag{1}$$

(b) *computing the rth column of L*

$$l_{ir} = \frac{a_{ir} - \sum\limits_{k=\max(1,i-p,r-p)}^{r-1} l_{ik}u_{kr}}{u_{rr}} \quad (i = r+1, \dots, r+p); \tag{2}$$

2. *when $r = n, n-1, \dots, j+p$*
(1) $r = n$

$$u_{ir} = a_{ri} \quad (i = n-p, \dots, n), \qquad l_{ri} = \frac{a_{ir}}{u_{rr}} \quad (i = n-p, \dots, n-1);$$

(2) $r = n-1, \ldots, j+p$
(a) *computing the* r*th row of* U

$$u_{ir} = a_{ri} - \sum_{k=r+1}^{\min(n,i+p,r+p)} l_{kr}u_{ik} \quad (i = r, \ldots, r-p); \tag{3}$$

(b) *computing the* r*th column of* L

$$l_{ri} = \frac{a_{ir} - \sum\limits_{k=r+1}^{\min(n,i+p,r+p)} l_{ki}u_{rk}}{u_{rr}} \quad (i = r-1, \ldots, r-p); \tag{4}$$

3. *when* $r = j+p-1, \ldots, j+1, j$
(1) *computing the* r*th row of* U

$$u_{ir} = a_{ri} - \sum_{k=r+1}^{\min(n,i+p,r+p)} l_{kr}u_{ik} - \sum_{k=\max(1,r-p,i-p)}^{j-1} l_{rk}u_{ki} \quad (i = r, r-1, \ldots, j); \tag{5}$$

(2) *computing the* r*th column of* L

$$l_{ri} = \frac{a_{ir} - \sum\limits_{k=r+1}^{\min(n,i+p,r+p)} l_{ki}u_{rk} - \sum\limits_{k=\max(1,r-p,i-p)}^{j-1} l_{ik}u_{kr}}{u_{rr}} \quad (i = r-1, \ldots, j). \tag{6}$$

Proof. The three cases regarding the formulae for computing $\{l_{ij}\}$ and $\{u_{ij}\}$ may be similarly solved.

1. For the first case, when $r = 1$, the initial values are derived:

$$u_{1i} = a_{1i}(i = 1, \ldots, p+1) \quad \text{and} \quad l_{i1} = \frac{a_{i1}}{u_{11}}(i = 2, \ldots, p+1).$$

When $r = 2, \ldots, j-1$, multiplying the rth row of L_j with the ith column of U_j, we have

$$u_{ri} + \sum_{k=\max(1,i-p,r-p)}^{r-1} l_{rk}u_{ki} = a_{ri}(i = r, \ldots, r+p),$$

so we have Eq. (1), i.e. the rth row of U_j is obtained; multiplying the rth column of U_j with ith row of L_j, we have

$$l_{ri}u_{rr} + \sum_{k=\max(1,r-p,i-p)}^{j-1} l_{ik}u_{kr} = a_{ir}(i = r+1, \ldots, r+p),$$

so we have Eq. (2), i.e. the rth column of L_j is obtained. Performing the above process, each column of L_j and each row of U_j may be obtained in turn respectively. Note that each step is always based on the result obtained in the former step.

2. The second case may be similarly obtained. Different from the first case, the process begins with $r = n$ and iterates forward. From $r = n-1$ to $j+p$, the rth row of U_j and the rth column of L_j are given in turn. When $r = n$, the initial value are:

$$u_{in} = a_{ni}(i = n-p, \ldots, n) \quad \text{and} \quad l_{ni} = \frac{a_{in}}{u_{nn}}(i = n-1, \ldots, n-p).$$

3. The third case is about the central rows and columns L_j and U_j. By using the results of the above two cases, it may also be obtained when iterating forward from $r = j+p-1$ to $r = j$. For the rth row of U_j, multiplying the rth row of L_j with ith ($i = r, r-1, \ldots, j$) column of U_j, we have

$$u_{ir} + \sum_{k=r+1}^{\min(n,i+p,r+p)} l_{kr}u_{ik} + \sum_{k=\max(1,r-p,i-p)}^{j-1} l_{rk}u_{ki} = a_{ri}.$$

For the rth column of L_j, multiplying the rth column of U_j with ith ($i = r-1, \ldots, j$) row of L_j, we have

$$l_{ri}u_{rr} + \sum_{k=r+1}^{\min(n,i+p,r+p)} l_{ki}u_{rk} + \sum_{k=\max(1,r-p,i-p)}^{j-1} l_{ik}u_{kr} = a_{ir}.$$

So we have Eq. (5), i.e. the rth row of U_j and Eq. (6), i.e. rth column of L_j is obtained ($r = j+p-1, \ldots, j+1, j$) in order starting with the $r = j+p-1$. $\square$

Theorem 2.2. *Let $A = (a_{ij})$ be a nonsingular equal bandwidth matrix of order n and $A^{-1} = X = (x_{ij})$. Then the jth ($j = 1, 2, \dots, n$) column elements of X may be obtained with the following formulae:*

1. $i = j, j+1, \dots, j+p-1$,*i.e.the initial value:*

$$x_{jj} = \frac{1}{u_{jj}};$$
$$x_{ij} = \frac{-(u_{ji}x_{jj} + u_{j+1,i}x_{j+1,j} + \cdots + u_{i-1,i}x_{i-1,j})}{u_{ii}};$$

2. $i = j-1, \dots, 2, 1$,

$$x_{ij} = \frac{-(u_{i,i+1}x_{i+1,j} + u_{i,i+2}x_{i+2,j} + \cdots + u_{i,i+p}x_{i+p,j})}{u_{ii}};$$

3. $i = j+p, \dots, n$,

$$x_{ij} = \frac{-(u_{i-p,i}x_{i-p,j} + \cdots + u_{i-2,i}x_{i-2,j} + u_{i-1,i}x_{i-1,j})}{u_{ii}}.$$

Proof. We denote the jth column vector of X by X_j and the jth fundamental vector of R^n by $e_j = (0, \dots, 0, 1, 0, \dots, 0)^{\mathrm{T}}$ ($j = 1, 2, \dots, n$). By the jth twisted decomposition in Theorem 2.1, we have

$$L_jU_jX_j = e_j.$$

By the structure of L_j, it is clear that

$$L_je_j = e_j.$$

Combining the above two equalities, we have

$$U_jX_j = e_j.$$

Solving this system, the initial value may be derived first. For the second case, $i < j$, we have forward substitution. The third case, $i > j$, involves backward substitution. the third case follows when substituting backwards. □

If A is symmetric banded matrix, there is the decomposition $A = LDL^{\mathrm{T}}$, where L is a lower triangle matrix, D is a diagonal matrix, see [12, p. 265]. Then the following two theorems may be given from Theorems 2.1 and 2.2.

Theorem 2.3. *Let $A = (a_{ij})$ be nonsingular symmetric equal bandwidth matrix of order n. For $j = 1, 2, \dots, n$,*

(i) *when $j = 1$, $A = L^{\mathrm{T}}DL$; when $j = n$, $A = LDL^{\mathrm{T}}$;*
(ii) *when $j = 2, \dots, n-1$,there exists a twisted decomposition such that*

$$A = L_jD_jL_j^{\mathrm{T}},$$

where L_j and $D_j = \mathrm{diag}(d_1, d_2, \dots, d_n)$ may be obtained with the formulae:

1. *when $r = 1, 2, \dots, j-1$*

$$d_r = a_{ri} - \sum_{k=\max(1,i-p,r-p)}^{r-1} l_{rk}d_kl_{ik}$$
$$l_{ir} = \left(a_{ir} - \sum_{k=\max(1,i-p,r-p)}^{r-1} l_{ik}d_kl_{rk}\right) \Big/ d_r \quad (i = r+1, \dots, r+p);$$

2. *when $r = n, n-1, \dots, j+p$*

$$d_r = a_{rr} - \sum_{k=r+1}^{\min(n,i+p,r+p)} l_{kr}^2d_k$$
$$l_{ri} = \left(a_{ir} - \sum_{k=r+1}^{\min(n,i+p,r+p)} l_{ki}d_kl_{kr}\right) \Big/ d_r \quad (i = r-1, \dots, r-p);$$

3. *when* $r = j + p - 1, \dots, j + 1, j$

$$d_r = a_{ri} - \sum_{k=r+1}^{\min(n,i+p,r+p)} l_{kr}^2 d_k - \sum_{k=\max(1,r-p,i-p)}^{j-1} l_{rk}^2 d_k$$

$$l_{ri} = \left(a_{ir} - \sum_{k=r+1}^{\min(n,i+p,r+p)} l_{ki} d_k l_{kr} - \sum_{k=\max(1,r-p,i-p)}^{j-1} l_{ik} d_k l_{rk} \right) \Big/ d_r \quad (i = r-1, \dots, j).$$

For the symmetric banded matrix, it is only needed to determine the elements under the main diagonal of the inverse matrix, so we have the following theorem.

Theorem 2.4. *Let $A = (a_{ij})$ be a nonsingular symmetric equal bandwidth matrix of order n and $A^{-1} = X = (x_{ij})$. Then the jth $(j = 1, 2, \dots, n)$ column elements of X may be computed in the following formulae:*

1. *for $i = j, j + 1, \dots, j + p - 1$, i.e. the initial value:*

$$x_{jj} = 1/d_j, \qquad x_{ij} = -(l_{ij} x_{jj} + l_{i,j+1} x_{j+1,j} + \dots + l_{i,i-1} x_{i-1,j});$$

2. *for $i = j + p, \dots, n - 1, n$*

$$x_{ij} = -(l_{i,i-p} x_{i-p,j} + \dots + l_{i,i-2} x_{i-2,j} + l_{i,i-1} x_{i-1,j}).$$

Then, a method for the inverse of the equal bandwidth matrix is presented, which finds the inverse elements of the matrix A by column in turn.

3. The computing complexity

The arithmetic operation count for the method proposed to find an inverse of a banded matrix of order n is made by the following two steps:

(1) The n twisted decompositions. It may be implemented by the following process:

First, let $j = 1$, $L_1 U_1 = UL$, then $2p(p + 1)n$ flops are required. Then, the jth decomposition $(j = 2, \dots, n)$, for the top rows and columns and for the bottom rows and columns of L_j and U_j, keeps the values of the $(j - 1)$th decomposition; only updating the $(j-1)$th column of L_j and the $(j-1)$th row of U_j, and the central rows of U_j and columns of L_j. So $2p(p+1)n+k(p)$ flops are required, where $k(p)$ is a constant related to p.

The total count for n twisted decompositions is therefore $4p(p + 1)n + k(p)$ flops.

(2) The n column of the inverse matrix:

$$2pn^2 - p(p - 1)n.$$

So the total arithmetic operation is

$$2pn^2 + (3p + 5)pn + k(p) \text{ flops, i.e., } 2pn^2 + O(n).$$

The standard technique for finding the inverse of the banded matrices of order n is based on the LU decomposition of the banded matrix A. After the decomposition is carried out, the jth $(j = 1, 2, \dots, n)$ column of the inverse matrix may be obtained when we solve the following linear systems

$$\begin{cases} LY_j = e_j, \\ UX_j = Y_j. \end{cases}$$

Where e_j is the jth column of the identity matrix, X_j is the jth column of the inverse matrix, Y_j is an intermediate vector. For convenience, it is denoted with LU method. The arithmetic operation count for LU method is $(4p - 1)n^2 + O(n)$.

From the above analysis, the method in this paper is about 2 times faster than the standard method based on the LU decomposition. This is a significant improvement on the above LU method.

4. Application to tridiagonal and pentadiagonal matrix

4.1. Tridiagonal matrix

Assume that the tridiagonal matrices under consideration are in the form

$$A = \begin{pmatrix} b_1 & c_1 & & & \\ a_2 & b_2 & c_2 & & \\ & \ddots & \ddots & \ddots & \\ & & a_{n-1} & b_{n-1} & c_{n-1} \\ & & & a_n & b_n \end{pmatrix} \tag{7}$$

and denote it by $A = \operatorname{diag}(a_i, b_i, c_i)$. Throughout the paper, let its principal minors be nonzero.

For the matrix A, a formulae for the inverse is given in term of the principal minors, see [8]. This is an important result and many researches for the inverse refer to it.

Lemma 4.1 *([8]). Assume that A is nonsingular, let $A^{-1} = X = (x_{ij})$, then the entries of A^{-1} are given by*

$$x_{ij} = \begin{cases} (-1)^{i+j} c_i c_{i+1} \cdots c_{j-1} \theta_{i-1} \phi_{j+1}/\theta_n & i \le j, \\ (-1)^{i+j} a_{j+1} a_{j+2} \cdots a_i \theta_{i-1} \phi_{j+1}/\theta_n & i > j \end{cases}$$

where θ_i is the principal minors of A and satisfy

$$\theta_i = b_i\theta_{i-1} - a_i c_{i-1}\theta_{i-2} \ (i = 1, 2, \dots, n), \quad \theta_{-1} = 0, \quad \theta_0 = 1;$$
$$\phi_i = b_i\phi_{i+1} - a_{i+1} c_i \phi_{i+2} \ (i = n, n-1, \dots, 1), \quad \phi_{n+1} = 1, \quad \phi_{n+2} = 0.$$

In this section, the explicit expressions of the inverse are presented. and then it is proved that Lemma 4.1 is a consequence of the explicit inverse obtained. First, the twisted decompositions of the tridiagonal matrix, which are easily deduced from Theorem 2.1, are presented.

A tridiagonal matrix can be decomposed as $A = LU$, where L and U are bidiagonal matrices, also see [11, p. 95]. The decomposition $A = UL$ may be similarly given.

Lemma 4.2. *Let A be a tridiagonal matrix in the form (7). For each $j = 1, 2, \dots, n$,*

(i) *when $j = 1$, A=UL; when $j = n$, A=LU;*

(ii) *when $j = 2, \dots, n-1$, there exists a twisted decomposition such that*

$$A = L_j U_j = \begin{pmatrix} 1 & & & & & & \\ l_2 & 1 & & & & & \\ & \ddots & \ddots & & & & \\ & & l_j & 1 & l_{j+1} & & \\ & & & & \ddots & \ddots & \\ & & & & & 1 & l_n \\ & & & & & & 1 \end{pmatrix} \begin{pmatrix} d_1 & u_1 & & & & & \\ & \ddots & \ddots & & & & \\ & & d_{j-1} & u_{j-1} & & & \\ & & & d_j & & & \\ & & & u_j & d_{j+1} & & \\ & & & & \ddots & \ddots & \\ & & & & & u_{n-1} & d_n \end{pmatrix}$$

where the sequences $\{l_i\}$, $\{d_i\}$ and $\{u_i\}$ may be computed in the following formulae.

Case 1. $i < j$

$$u_i = c_i (i = 1, 2, \dots, j-1),$$
$$d_1 = b_1, \quad l_i = a_i/d_{i-1}, \quad d_i = b_i - l_i u_{i-1} (i = 2, \dots, j-1).$$

Case 2. $i > j$

$$u_i = a_{i+1} (i = n-1, \dots, j+1),$$
$$d_n = b_n, \quad l_i = c_{i-1}/d_i (i = n, \dots, j+1),$$
$$d_i = b_i - l_{i+1} u_i (i = n-1, \dots, j+1).$$

Case 3. $i = j$

$$l_i = a_i/d_{i-1}, \quad u_i = a_{i+1} d_i = b_i - l_i u_{i-1} - l_{i+1} u_i.$$

Similar to Theorem 2.2, it is easy to give the following theorem about the inverse of a tridiagonal matrix, which recursively computes the elements each column of the inverse.

Theorem 4.3. *Let $A = \mathrm{diag}(a_i, b_i, c_i)$ be a tridiagonal matrix in the form (7), Let $A^{-1} = X = (x_{ij})$, then the jth ($j = 1, 2, \dots, n$) column elements of X may be obtained in the following formulae*

$$x_{jj} = 1/d_j, \quad x_{ij} = -\frac{u_i x_{i+1j}}{d_i} \quad (i = j-1, \dots, 1), \quad x_{ij} = -\frac{u_{i-1} x_{i-1j}}{d_i} \quad (i = j+1, \dots, n),$$

where $\{d_i\}$ and $\{u_i\}$ are the sequences in Lemma 4.2.

From the recurrence relation in Theorem 4.3, and notice that $u_i = c_i (i < j)$ and $u_i = a_{i+1} (i > j)$, we have the following Theorem about the expression of the elements of the inverse.

Theorem 4.4. *Let $A = \operatorname{diag}(a_i, b_i, c_i)$ be a tridiagonal matrix in the form (7). Let $A^{-1} = X = (x_{ij})$, then the elements of the inverse of A may be expressed as*

$$x_{ij} = \begin{cases} (-1)^{j-i} \dfrac{c_i \cdots c_{j-1}}{d_i \cdots d_{j-1} d_j} & i \le j \\ (-1)^{i-j} \dfrac{a_{j+1} \cdots a_i}{d_j \cdots d_{i-1} d_i} & i > j \end{cases}$$

where $\{d_i\}$ are the sequences obtained in Lemma 4.2.

The explicit inverse of a tridiagonal matrix in Lemma 4.1 is the consequence of Theorem 4.4.
For a fixed $j(j = 1, 2, \ldots, n)$, if $k \le j$, we set

$$d_k = \frac{\theta_k}{\theta_{k-1}}, \quad \theta_{-1} = 0, \qquad \theta_0 = 1, \tag{8}$$

From the case 1 in Lemma 4.2, we get the recurrence relation

$$\theta_k = b_k \theta_{k-1} - a_k c_{k-1} \theta_{k-2} \quad (k = 1, 2, \ldots, j-1).$$

If $k > j$, we set

$$d_k = \frac{\phi_k}{\phi_{k+1}}, \quad \phi_{n+1} = 1, \quad \phi_{n+2} = 0. \tag{9}$$

From the case 2 in Lemma 4.2, we get the recurrence relation

$$\phi_k = b_k \phi_{k+1} - a_{k+1} c_k \phi_{k+2} \quad (k = n, n-1, \ldots, j+1).$$

From Theorem 4.4 and the relations (8) and (9), we get

$$x_{ij} = \begin{cases} (-1)^{j-i} \dfrac{c_i \cdots c_{j-1}}{d_i \cdots d_{j-1} d_j} = (-1)^{i+j} c_i \cdots c_{j-1} \dfrac{(d_1 \cdots d_{i-1})(d_{j+1} \cdots d_n)}{d_1 \cdots d_n} & i \le j, \\ (-1)^{i-j} \dfrac{a_{j+1} \cdots a_i}{d_j \cdots d_{i-1} d_i} = (-1)^{i+j} a_{j+1} \cdots a_i \dfrac{(d_1 \cdots d_{j-1})(d_{i+1} \cdots d_n)}{d_1 \cdots d_n} & i > j. \end{cases}$$

Notice that $\theta_n = d_1 \cdots d_n = \det A$. As a consequence, we achieve

$$x_{ij} = \begin{cases} (-1)^{i+j} c_i c_{i+1} \cdots c_{j-1} \theta_{i-1} \phi_{j+1} / \theta_n & i \le j, \\ (-1)^{i+j} a_{j+1} a_{j+2} \cdots a_i \theta_{i-1} \phi_{j+1} / \theta_n & i > j. \end{cases}$$

4.2. Pentadiagonal Toeplitz matrix

Assume that the pentadiagonal Toeplitz matrix under consideration is in the form

$$M = \begin{pmatrix} x & y & v & & & & \\ z & x & y & v & & & \\ w & z & x & y & v & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots & \ddots & v \\ & & & \ddots & \ddots & x & y \\ & & & & w & z & x \end{pmatrix}. \tag{10}$$

This kind of matrix often arises in many problems, for example numerical solution of differential equation. Throughout the paper, let it˙s principal minors be nonzero.

Apparently, this matrix is a banded matrix with the bandwidth $p = 2$, so Theorems 2.1 and 2.2 hold true for it.

For convenience, write the jth decomposition of the pentadiagonal matrix M as

$$M = L_j D_j^{-1} U_j, \tag{11}$$

where

$$L_j = \begin{pmatrix} d_1 &&&&&&&& \\ l_2 & d_2 &&&&&&& \\ w & l_3 & d_2 &&&&&& \\ & \ddots & \ddots & \ddots &&&&& \\ && w & l_j & d_j & l_{j+1} & v && \\ &&&&& d_{j+1} & \ddots & \ddots & \\ &&&&&& \ddots & \ddots & v \\ &&&&&&& \ddots & l_n \\ &&&&&&&& d_n \end{pmatrix}$$

$$U_j = \begin{pmatrix} d_1 & u_1 & v &&&&&& \\ & \ddots & \ddots & \ddots &&&&& \\ && d_{j-1} & u_{j-1} & v &&&& \\ &&& d_j &&&&& \\ &&& u_j & d_{j+1} &&&& \\ &&& w & u_{j+1} & d_{j+2} &&& \\ &&&& \ddots & \ddots & \ddots && \\ &&&&& \ddots & \ddots & \ddots & \\ &&&&&& w & u_{n-1} & d_n \end{pmatrix}$$

and $D_j = \operatorname{diag}\left(d_1, \dots, d_j, \dots, d_n\right)$. The formulae for computing the sequences $\{l_i\}$, $\{d_i\}$ and $\{u_i\}$ can be similarly given from Theorem 2.1 with little modification. According to Theorem 2.2, the following Theorem 4.5, which is the recurrence relation of the entries of the inverse of the matrix M, is easily obtained.

Theorem 4.5. *Let M be a nonsingular pentadiagonal matrix of order n and $M^{-1} = X$. Denote the jth $(j = 1, 2, \dots, n)$ column vector of X by*

$$\boldsymbol{x} = \begin{pmatrix} x_1 & \cdots & x_{j-1} & x_j & x_{j+1} & x_{j+2} & \cdots & x_n \end{pmatrix}^{\mathrm{T}},$$

then the vector $\boldsymbol{x}$ may be obtained from the following formulae:

1. *the initial value:*

$$x_j = 1/d_j, \quad x_{j+1} = -u_j x_j / d_{j+1};$$

2. $i = j + 2, \dots, n$

$$x_i = -\frac{u_{i-1}}{d_i} x_{i-1} - \frac{w}{d_i} x_{i-2}; \tag{12}$$

3. $i = j - 1, \dots, 2, 1$

$$x_i = -\frac{u_i}{d_i} x_{i+1} - \frac{v}{d_i} x_{i+2}. \tag{13}$$

So the entries of the inverse of the matrix M are determined by the second order linear homogeneous difference equation with variable coefficients (12) when $i = j + 2, \dots, n$ and the Eq. (13) when $i = j - 1, \dots, 2, 1$.

The solution of a second order linear homogeneous difference equation with variable coefficients is given by R. K. Mallik in [13]; for the nonhomogeneous case, the solution is also given by R. K. Mallik in [14], and the result is applied to give the explicit inverse of a tridiagonal matrix.

Here, we use the results given in [13], and give the explicit expression of the entries of the inverse of the matrix M. Before giving the inverse, we have to introduce a notions about $S_q(L, U)$.

Let N denote the set of natural numbers. A set $S_q(L, U)$, where $q, L, U \in \mathrm{N}$, has been defined in [13] as the set of q-tuples with elements from $\{L, L+1, \dots, U\}$ arranged in ascending order so that no two consecutive elements are present:

$$\begin{aligned} S_q(L, U) &\triangleq \{L, L+1, \dots, U\} \quad \text{if } U \geq L \text{ and } q = 1, \\ &\triangleq \left\{\left(k_1, \dots, k_q\right) : k_1, \dots, k_q \in \{L, L+1, \dots, U\}\,;\, k_l - k_{l-1} \geq 2 \text{ for } l = 2, \dots, q\right\} \end{aligned}$$

if $U \geq L + 2$ and $2 \leq q \leq \left\lfloor \frac{U-L+2}{2} \right\rfloor$,
$= \emptyset$ otherwise.

For the case $i = j+2, \ldots, n$, rewrite the relation (12) as

$$x_{i+2} = -\frac{u_{i+1}}{d_{i+2}}x_{i+1} - \frac{w}{d_{i+2}}x_i \quad (i = j, j+1, \ldots, n-2),$$

and define

$$A_i = \frac{u_{i+1}}{d_{i+2}}, \qquad B_i = \frac{w}{d_{i+2}},$$

$$\sigma_k = \frac{B_k}{A_{K-1}A_k} = \frac{wd_{k+1}}{u_k u_{k+1}} \quad (k = j+1, \ldots, n-2), \qquad \sigma_j = \frac{B_j}{A_{n-2}A_j} = \frac{wd_n}{u_{n-1}u_{j+1}}.$$

From Proposition 5 in [13], the solution of the difference equation (12) with initial x_j, x_{j+1} is

$$x_i = C_{i-2}x_{j+1} + D_{i-2}x_j \quad (i \geq j+1),$$

where

$$C_{j-1} = 1, \quad C_j = -A_j$$
$$D_{j-1} = 0, \quad D_j = -B_j, \quad D_{j+1} = B_j A_{j+1}.$$

And denote $m = i - j + 1$. For $i \geq j+1$,

$$C_i = (-1)^m \left(A_j \cdots A_i\right) \left(1 + \sum_{q=1}^{\lfloor (m)/2 \rfloor} (-1)^q \sum_{(k_0, \ldots, k_q - 1)} \left(\sigma_{k_0} \cdots \sigma_{k_{q-1}}\right)\right).$$

where

$$\sigma_{k_0} \cdots \sigma_{k_{q-1}} = w^q (-1)^q \prod_{s=0}^{q} -1 \frac{d_{k_s+1}}{u_{k_s}u_{k_s+1}}$$
$$\left(k_s = j + l_s - 1, \left(l_0, \ldots, l_{q-1}\right) \in S_q(2, m)\right);$$

for $i \geq j+2$,

$$D_i = (-1)^{m+1} B_j \left(A_{j+1} \cdots A_i\right) \left(-1 + \sum_{q=2}^{\lfloor (m+1)/2 \rfloor} (-1)^q \sum_{(k_1, \ldots, k_{q-1}) \in S_{q-1}(3, m+1)} \left(\sigma_{k_1} \cdots \sigma_{k_{q-1}}\right)\right)$$

where

$$\sigma_{k_1} \cdots \sigma_{k_{q-1}} = w^{q-1} (-1)^{q-1} \prod_{s=1}^{q-1} \frac{d_{k_s+1}}{u_{k_s}u_{k_s+1}}$$
$$\left(k_s = j + l_s - 1, \left(l_1, \ldots, l_{q-1}\right) \in S_{q-1}(3, m+1)\right).$$

For the case $i = j-1, \ldots, 2, 1$, denote $y_i = x_{j+2-i}$ $(i = 1, 2, \ldots, j+1)$, the difference equation (13) becomes

$$y_i = -\frac{u_{j+2-i}}{d_{j+2-i}}y_{i-1} - \frac{v}{d_{j+2-i}}y_{i-2}, \quad (i = 3, \ldots, j+1)$$

with the initial value $y_1 = x_{j+1}, y_2 = x_j$. Rewrite the above recurrence relation:

$$y_{i+2} = -\frac{u_{j-i}}{d_{j-i}}y_{i+1} - \frac{v}{d_{j-i}}y_i, \quad (i = 1, 2, \ldots, j-1). \tag{14}$$

Define

$$A_i = \frac{u_{j-i}}{d_{j-i}}, \qquad B_i = \frac{v}{d_{j-i}} \quad (i = 1, 2, \ldots, j-1),$$

$$\sigma_k = \frac{B_k}{A_{K-1}A_k} = \frac{vd_{j-k}}{u_{j-k+1}u_{j-k}} \quad (k = 2, \ldots, j-1), \qquad \sigma_1 = \frac{B_1}{A_{j-1}A_1} = \frac{vd_1}{u_1 u_{j-1}}.$$

From Proposition 5 in [13], the solution of the difference equation (14) is

$$y_i = C_{i-2}y_2 + D_{i-2}y_1, \quad (i = 2, 3, \ldots, j+1)$$

where

$$C_0 = 1, \quad C_1 = -A_1$$
$$D_0 = 0, \quad D_1 = -B_1, \quad D_2 = B_1 A_2$$

Table 1
Comparison of the two methods in the case of non-symmetry.

N	p	$T_{LU}(\mathrm{s})$	$T_{LjUj}(\mathrm{s})$	ERR_{LU}	ERR_{LjUj}
	10	2.0770	1.1010	7.5675e−15	7.6247e−15
1000	20	3.3866	1.9642	9.8119e−15	1.0005e−14
	30	4.4417	2.6206	1.1464e−14	1.1523e−14
	10	4.5412	2.7792	9.3162e−15	9.2681e−15
1500	20	6.9110	4.0466	1.2118e−14	1.2088e−14
	30	9.4812	5.5939	1.4654e−14	1.4740e−14
	10	9.8467	5.2704	1.0688e−14	1.0685e−14
2000	20	12.236	7.2192	1.4112e−14	1.3978e−14
	30	16.968	10.0140	1.6420e−14	1.6351e−14

and

$$C_i = (-1)^i (A_1 \cdots A_i) \left(1 + \sum_{q=1}^{\lfloor i/2 \rfloor} (-1)^q \sum_{(k_0,\ldots,k_{q-1}) \in S_q(2,i)} \left(\sigma_{k_0} \cdots \sigma_{k_{q-1}} \right) \right) \quad \text{for } i \geq 2$$

$$D_i = (-1)^{i+1} B_1 (A_2 \cdots A_i) \left(-1 + \sum_{q=2}^{\lfloor (i+1)/2 \rfloor} (-1)^q \sum_{(k_1,\ldots,k_{q-1}) \in S_{q-1}(3,i)} \left(\sigma_{k_1} \cdots \sigma_{k_{q-1}} \right) \right) \quad \text{for } i \geq 3.$$

So, in the case of $i < j$, i.e., $i = j - 1, \ldots, 2, 1$, the entries of the inverse are

$$x_{j+2-i} = C_{i-2} y_2 + D_{i-2} y_1 \quad (i = 2, \ldots, j+1),$$

when i is from 2 to $j + 1$, the values of $x_j, x_{j-1}, \ldots, x_1$ are given.

5. Numerical experiments

We have used MATLAB in a PC to make experiments about the inverses of banded matrices with the two methods: the *LU* method and the method in this paper. The experiment results are shown in the following tables, where N is the dimension of the banded matrix, p is the bandwidth. T_{LU} and T_{LjUj} denote the time cost by *LU* method and the method in this paper respectively; ERR_{LU} and ERR_{LjUj} denote the error of the inverse of *LU* method and the method in this paper respectively.

It will be seen from the following experimental results that the error of this method proposed is much smaller; and the time cost for the method in this paper is much smaller than that of the *LU* method.

Example 5.1. The banded matrices are generated by MATLAB. In MATLAB, we first generate a random matrix of order n with the function rand(n), i.e. $A = (a_{ij}) = \mathrm{rand}(n)$, then put $a_{ij} = 0$ if $|i - j| > p$, and set $a_{ii} = \sum_{k=r-p}^{r+p} a_{ij}$. So the matrix A is nonsymmetric and strictly diagonally dominant. With the *LU* method and the method in this paper, the inverses of the test matrices are presented. The experiment results are shown in Table 1.

Example 5.2. Consider the Poisson equation

$$\begin{cases} \dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2} = G(x, y), \quad (x, y) \in R, \\ u(x, y)|_{\Gamma} = g(x, y) \end{cases}$$

where R is: $0 < x, y < 1$, Γ is the boundary of R ([15, p. 90]).

Solving the equation with the finite difference method. Dividing the area $0 \leq x, y \leq 1$ with the square grid, i.e. $0 = x_0 < x_1 < \cdots < x_n = 1$, $0 = y_0 < y_1 < \cdots < y_n = 1$, where $x_i = ih, y_j = jh (i, j = 0, 1, \ldots, n)$, $h = 1/n$. Denote the node (x_i, y_j) by (i, j). So discretizing the equation with the initial value condition, and then getting algebraic equations $Au = f$:

$$\begin{cases} 4u_{ij} - u_{i+1,j} - u_{i-1,j} - u_{i,j+1} - u_{i,j-1} = -h^2 G_{ij} \\ (i = 1, 2, \ldots, n-1, j = 1, 2, \ldots, n-1) \end{cases},$$

where the coefficient matrix A is a symmetric banded matrix of order $N = (n - 1)^2$, with bandwidth $p = n - 1$. With *LU* method and the method proposed in this paper, the inverses of the matrix A are presented. The experiment results are shown in Table 2.

Example 5.3. Consider the two dimension heat conduction equation:

$$\begin{cases} \dfrac{\partial u}{\partial t} = \dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2}, \quad (0 < t \leq T, 0 < x, y < 1) \\ u(x, y, 0) = \varphi(x, y) \quad 0 < x, y < 1 \\ u(0, y, t) = u(1, y, t) = u(x, 0, t) = u(x, 1, t) = 0. \end{cases}$$

Table 2
Comparison of the two methods about a symmetric banded matrix,

$n-1$	$N=(n-1)^2$	p	$T_{LU}(s)$	$T_{LjUj}(s)$	ERR_{LU}	ERR_{LjUj}
20	400	20	0.3904	0.2090	4.0296e−14	3.9690e−14
25	625	25	0.9575	0.6034	6.4900e−14	6.5266e−14
30	900	30	2.1991	1.6187	1.0086e−13	9.9933e−14
35	1225	35	4.4731	3.2361	1.4746e−13	1.4549e−13
40	1600	40	8.5280	5.0029	2.0430e−13	2.0558e−13
45	2025	45	14.9300	8.4320	2.7205e−13	2.8185e−13
50	2500	50	25.7520	15.3520	3.5480e−13	3.5809e−13

Table 3
Comparison of the two methods about a pentadiagonal Toeplitz matrix.

N	$T_{LU}(s)$	$T_{LjUj}(s)$	ERR_{LU}	ERR_{LjUj}
500	0.1960	0.1156	4.7323e−15	6.4332e−15
800	0.4210	0.2530	5.8895e−15	8.1322e−15
1000	0.5960	0.3493	6.5484e−15	9.0901e−15
1500	1.5290	0.9690	7.9604e−15	1.1130e−14
2000	2.5780	1.6260	9.1572e−15	1.2850e−14
2500	4.0300	2.5160	1.0215e−14	1.4365e−14
3000	6.2040	3.6070	1.1173e−14	1.5735e−14

Table 4
Comparison of the two methods about a tridiagonal matrix.

N	T_{LU} (s)	T_{LjUj} (s)	ERR_{LU}	ERR_{LjUj}
200	0.0630	0.0310	4.6127e−16	2.9798e−15
500	0.2800	0.1570	4.8124e−16	4.8764e−15
1000	1.0780	0.6570	5.1281e−16	6.9723e−15
1500	2.2820	1.3610	5.4254e−16	8.5701e−15
2000	3.7150	2.1060	5.7073e−16	9.9137e−15
2500	7.4150	4.1820	5.9759e−16	1.1096e−15
3000	9.6540	5.2160	6.2329e−16	1.2163e−15

For convenience, the steps in x and y direction are equal, i.e, $\Delta x = \Delta y = h$, the step in the t direction is l. Let node be $\left(x_i, y_j, t_k\right)$, where $x_i = ih$, $y_j = jh$, $t_k = kl$. Solving the equation with the finite difference method, the classical inexplicit difference scheme:

$$(1+4r)\, u_{i,j}^{k+1} - r\left(u_{i+1,j}^{k+1} + u_{i-1,j}^{k+1} + u_{i,j+1}^{k+1} + u_{i,j-1}^{k+1}\right) = u_{i,j}^{k}$$

where $r = l/h^2$. So, the nodes of the $(k+1)$ layer can be given by an algebraic equations: $Mu = f$, where M is a symmetric pentadiagonal Toeplitz matrix.

Set $r = 1$, with LUmethod and the method proposed in this paper, the inverses of the matrix A are presented. The experimental results are shown in Table 3.

Example 5.4. In this example, the following tridiagonal matrix

$$A = \begin{pmatrix} 4 & 2 & & & \\ 1 & 4 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 4 & 1 \\ & & & 2 & 4 \end{pmatrix},$$

which often comes in spline interpolation under some boundary conditions, is made an example to compare the method in this paper with the LU method. The experiment results are shown in Table 4.

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